Coherent and incoherent dynamic structure functions of the free Fermi gas

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Abstract

A detailed calculation of the coherent and incoherent dynamic structure functions of the free Fermi gas, starting from their expressions in terms of the one- and semi–diagonal two–body density matrices, is derived and discussed. Their behavior and evolution with the momentum transfer is analyzed, and particular attention is devoted to the contributions that both functions present at negative energies. Finally, an analysis of the energy weighted sum rules satisfied by both responses is also performed. Despite of the simplicity of the model, some of the conclusions can be extended to realistic systems.

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Recent measurements of the dynamic structure function $S(q,\omega)$ in pure liquid ^{4}He and ^{3}He, and ^{3}He–^{4}He mixtures at high and low momentum transfer [1],[2],[3] have revived the interest in the theoretical analysis of $S(q,\omega)$ on both boson and fermion systems [3],[4],[5],[7] It is well known that at high momentum transfer q the scattering simplifies and only the incoherent part of the response survives. Therefore, splitting $S(q,\omega)$ in coherent and incoherent terms may help to understand its nature. The main purpose of this letter is to analyze both responses for the free Fermi gas at any value of q. In this case they can be calculated exactly because the Hamiltonian is easily diagonalized. Despite the simplicity of the model, it can be useful to understand certain features of the response in real systems like ^{3}He.

The dynamic structure function of a quantum system of N identical particles at zero temperature is defined as the probability of coupling the ground state to all states compatible with a momentum and energy transfer (q,ω) after a density fluctuation $\rho_q = \sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r_j}}$ takes place

$$S(q,\omega) = \frac{1}{N}\sum_{\{n\}} |\langle n \mid \rho_q \mid 0\rangle|^2\, \delta(E_n - E_0 - \omega) \tag{1}$$

The Fourier transform of $S(q,\omega)$ generates the density–density correlation factor $S(q,t)$ [6], which is the sum of the incoherent and coherent density responses [7]. These functions are defined as

$$S_{inc}(q,t) = \frac{1}{N}\sum_{j=1}^{N}\langle e^{-i\mathbf{q}\cdot\mathbf{r_j}} e^{iHt} e^{i\mathbf{q}\cdot\mathbf{r_j}} e^{-iHt}\rangle \tag{2}$$

$$S_{coh}(q,t) = \frac{1}{N}\sum_{i\neq j}^{N}\langle e^{-i\mathbf{q}\cdot(\mathbf{r_i}-\mathbf{r_j})} e^{-i\mathbf{q}\cdot\mathbf{r_j}} e^{iHt} e^{i\mathbf{q}\cdot\mathbf{r_j}} e^{-iHt}\rangle \tag{3}$$

where H and $\mathbf{r_j}$ are the Hamiltonian and the position operators, respectively. Notice that with the definition given in (3) only those terms where particles i and j are strictly different contribute to the coherent response, in contrast to other common definition where $S_{coh}(q,\omega)$ is taken as the whole density response and thus coincides with (1).

In a realistic interacting system, where the potential entering in H depends on the position of the particles, H is non–diagonal neither in momentum nor in configuration space, and the evaluation of the expectation values in Eqs. (1), (2) and (3) becomes a formidable problem. Different approximations have been deviced in the past, attempting to discern which are the leading contributions in the limits of high [8],[9] and low [10] momentum transfer. Even though

a considerable amount of information concerning the dynamics of quantum liquids and nuclear systems have been gatered using those methods, precise knowledge of the complete spectrum of the Hamiltonian is required if one seeks to calculate all three responses exactly.

One of the few systems for which all eigenvalues and eigenvectors of the Hamiltonian are known is the free Fermi gas, where H is diagonal in the momentum representation. In this case, the action of the momentum translation operators $\exp(i\mathbf{q} \cdot \mathbf{r_j})$ appearing in Eqs. (2) and (3) is straightforward

$$
\begin{aligned}
e^{-i\mathbf{q}\cdot\mathbf{r_j}}e^{iHt}e^{i\mathbf{q}\cdot\mathbf{r_j}}e^{-iHt} &= e^{-i\mathbf{q}\cdot\mathbf{r_j}}\exp\left[it\sum_{k=1}^{N}\frac{p_k^2}{2m}\right]e^{i\mathbf{q}\cdot\mathbf{r_j}}\exp\left[-it\sum_{l=1}^{N}\frac{p_l^2}{2m}\right] \\
&= \exp\left[it\left(\frac{(\mathbf{p_j}+\mathbf{q})^2}{2m}-\frac{p_j^2}{2m}\right)\right] \\
&= \exp\left[it\frac{q^2}{2m}\right]\exp\left[it\frac{\mathbf{q}\cdot\mathbf{p_j}}{m}\right]
\end{aligned}
\tag{4}
$$

and results in an exponential operator whose argument is linear in $\mathbf{p_j}$, thus yielding the position translation operator of particle j. After projecting on a complete basis of states in configuration space, the incoherent and coherent responses become functions of the one- and the semi–diagonal two–body density matrices

$$
S_{inc}(q,t) = e^{i\omega_q t}\frac{1}{\rho}\rho_1(vt) ,
\tag{5}
$$

$$
S_{coh}(q,t) = e^{i\omega_q t}\frac{1}{\rho}\int d\mathbf{r}\rho_2(\mathbf{r},0;\mathbf{r}+\mathbf{v}t,0)e^{i\mathbf{q}\cdot\mathbf{r}} ,
\tag{6}
$$

where ρ is the particle number density, $\mathbf{v} = \mathbf{q}/m$ is the recoiling velocity of particle j and $\omega_q = q^2/2m = mv^2/2$ its associated kinetic energy. Comparing to the $1/q$ series of the response derived by Gersch and coworkers in the early 70's, one readily notices that $S_{inc}(q,t)$ and $S_{coh}(q,t)$ are described by the first terms of the incoherent and coherent expansions, respectively. Higher order terms in the series are related to integrals of the potential and vanish when describing the response of a free system. As a consequence, the incoherent response of the free Fermi gas is entirely given by the Impulse Approximation (IA).

Due to the close relation between the one–body density matrix $\rho_1(x)$ and the momentum distribution $n(k)$, $S_{inc}(q,t)$ can be Fourier transformed to yield the standard representation of

the IA

$$S_{inc}(q,\omega) = \frac{\nu}{(2\pi)^3\rho}\int d\mathbf{k}\, n(k)\,\delta\left(\frac{(\mathbf{k}+\mathbf{q})^2}{2m} - \frac{k^2}{2m} - \omega\right) \tag{7}$$

$$= \frac{\nu m}{4\pi^2\rho q}\int_{|Y|}^{\infty} k\, n(k)\, dk, \tag{8}$$

$Y = m\omega/q - q/2$ being the West scaling variable and ν the degeneracy of each single–particle state of definite momentum. The momentum distribution of the free Fermi gas is a Heaviside step function $n(k) = \theta(k_F - k)$ that allows for the occupation of states up to the Fermi surface only. Therefore, the integral in Eq. (8) can be performed and the result, expressed in terms of a new set of dimensionless variables $\tilde{q} = q/k_F$ and $\tilde{\omega} = \omega/\epsilon_F$ with $\epsilon_F = k_F^2/2m$ the Fermi energy, is given by

$$S_{inc}(q,\omega) \equiv \frac{1}{\epsilon_F}S_{inc}(\tilde{q},\tilde{\omega}) = \frac{1}{\epsilon_F}\frac{3}{8\tilde{q}}\left[1 - \frac{1}{4}\left(\frac{\tilde{\omega}}{\tilde{q}} - \tilde{q}\right)^2\right]\theta\left[1 - \frac{1}{2}\left|\frac{\tilde{\omega}}{\tilde{q}} - \tilde{q}\right|\right] \tag{9}$$

which defines the dimensionless incoherent response $S_{inc}(\tilde{q},\tilde{\omega})$.

Proceeding in a similar way, the coherent response of the free Fermi gas can be brought to a form that closely resembles the IA

$$S_{coh}(q,\omega) = \frac{\nu}{(2\pi)^3\rho}\int d\mathbf{k}\, n(\mathbf{k},-\mathbf{q})\delta\left(\frac{(\mathbf{k}+\mathbf{q})}{2m} - \frac{k^2}{2m} - \omega\right) \tag{10}$$

where $n(\mathbf{k},\mathbf{q}))$ is the generalized momentum distribution introduced by Ristig and Clark

$$n(\mathbf{k},\mathbf{q}) = \frac{1}{\nu N}\rho\int d\mathbf{r_1}d\mathbf{r_1'}d\mathbf{r_2}\,\rho_2(\mathbf{r_1},\mathbf{r_2};\mathbf{r_{1'}},\mathbf{r_2})\,e^{i\mathbf{k}\cdot(\mathbf{r_1}-\mathbf{r_1'})}\,e^{-i\mathbf{q}\cdot(\mathbf{r_1}-\mathbf{r_2})} \tag{11}$$

$$= \frac{1}{\nu}\int d\mathbf{r}d\mathbf{r}'\,\rho_2(\mathbf{r},0;\mathbf{r}')\,e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\,e^{-i\mathbf{q}\cdot\mathbf{r}}\ . \tag{12}$$

Both the semi–diagonal two–body density matrix and the generalized momentum distribution of the non–interacting system are easily derived

$$\rho_2(\mathbf{r_1},\mathbf{r_2};\mathbf{r_1'},\mathbf{r_2}) = \rho^2\left[\ell(k_F r_{11'}) - \frac{1}{\nu}\ell(k_F r_{12})\ell(k_F r_{1'2})\right] \tag{13}$$

$$n(\mathbf{k},\mathbf{q}) = \theta(k_F - k)\left[(2\pi)^3\rho\delta(\mathbf{q}) - \theta(k_F - \|\mathbf{k}-\mathbf{q}\|)\right] \tag{14}$$

where $\ell(z)$ is the statistical correlation function, characteristic of fermion systems

$$\ell(z) = \frac{3}{z^3}\left[\sin z - z\cos z\right]\ . \tag{15}$$

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and therefore, inserting $n(\mathbf{k}, \mathbf{q})$ (14) in Eq.(10), the coherent response may be written as

$$S_{coh}(q, \omega) = \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{k}\, \theta(k_F - k) \left[(2\pi)^3 \rho\, \delta(\mathbf{q}) - \theta(k_F - \|\mathbf{k} - \mathbf{q}\|)\right] \delta\left(\frac{(\mathbf{k} + \mathbf{q})^2}{2m} - \frac{k^2}{2m} - \omega\right)$$
(16)

The $\delta(\mathbf{q})$ term in the integral contributes only at $q=0$, while the other carries all the information at finite values of the momentum transfer and can be evaluated analytically

$$S_{coh}(q, \omega) \equiv \frac{1}{\epsilon_F} S_{coh}(\tilde{q}, \tilde{\omega}) = \begin{cases} \left. \begin{array}{ll} -\frac{1}{\epsilon_F}\frac{3}{8\tilde{q}} \left[1 - \frac{1}{4}\left(\frac{\tilde{\omega}}{\tilde{q}} - \tilde{q}\right)^2\right] & \text{if } 0 \geq \tilde{\omega} \geq \tilde{q}^2 - 2\tilde{q} \\ -\frac{1}{\epsilon_F}\frac{3}{8\tilde{q}} \left[1 - \frac{1}{4}\left(\frac{\tilde{\omega}}{\tilde{q}} + \tilde{q}\right)^2\right] & \text{if } 2\tilde{q} - \tilde{q}^2 \geq \tilde{\omega} \geq 0 \end{array} \right\} & \text{for } \tilde{q} \leq 2 \\ \\ 0 & \text{for } \tilde{q} > 2 \end{cases}$$
(17)

thus defining the dimensionless coherent response $S_{coh}(\tilde{q}, \tilde{\omega})$.

Several conclusions on the behavior of the coherent and incoherent responses can be drawn from Equations (9) and (17), some of them being also valid for realistic interacting systems.

The incoherent response $S_{inc}(\tilde{q}, \tilde{\omega})$ of the free Fermi gas is positive defined for all energies between $\tilde{q}^2 - 2\tilde{q}$ and $\tilde{q}^2 + 2\tilde{q}$, and vanishes out of this range. At fixed $\tilde{q}$, $S_{inc}(\tilde{q}, \tilde{\omega})$ is a quadratic polynomial in $\tilde{\omega}$ with its maximum located at $\tilde{\omega} = \tilde{q}^2$, thus being symmetric around this point. Hence, both $S_{inc}(\tilde{q}, \tilde{\omega})$ and its derivatives are continuous.

At momentum transfer $\tilde{q} < 2$, $S_{coh}(\tilde{q}, \tilde{\omega})$ is non–zero and negative in the range $\tilde{\omega} \in (\tilde{q}^2 - 2\tilde{q}, 2\tilde{q} - \tilde{q}^2)$. It is split in two different parts, one defined at negative energies and the other at positive ones. At fixed $\tilde{q}$, both functions are quadratic polynomials in $\tilde{\omega}$ that differ only in the sign of the linear coefficient. This peculiarity gives rise to a symmetric and continuous $S_{coh}(\tilde{q}, \tilde{\omega})$ that, at $\tilde{\omega} = 0$, presents both a minimum and a discontinuity in the first derivative. At q's greater than twice the Fermi momentum, the coherent response vanishes.

The total response $S(\tilde{q}, \tilde{\omega})$, which is the sum of $S_{inc}(\tilde{q}, \tilde{\omega})$ (9) and $S_{coh}(\tilde{q}, \tilde{\omega})$ (17), is the well known Lindhard function [11],[12] that becomes totally incoherent at $\tilde{q} > 2$. At $\tilde{q}$'s smaller than 2, both the coherent and incoherent responses contribute and, even though they are of opposite sign in the free Fermi gas, the total response remains always positive. This is a general property of the dynamic structure function of all systems, as is apparent from Eq. (1). For instance, if at a certain energy one of the two responses is negative, its absolute value has to be smaller than the value of the other one at that point, which should be positive, as this is the only way to produce a total $S(q, \omega)$ that is either positive or zero.

This feature is particularly apparent at negative ω's, as the energy conserving delta appearing in the definition of $S(q, \omega)$ (Eq. (1)) forces the non–zero contributions to appear at positive energies only. The separation of the response in its coherent and incoherent terms breaks this constrain and both $S_{inc}(q, \omega)$ and $S_{coh}(q, \omega)$ can locate part of their strength at $\omega < 0$. However, as the total response is zero in this range, $S_{coh}(q, \omega)$ has to be equal to $-S_{inc}(q, \omega)$ at $\tilde{\omega} < 0$. This is once again a requirement for the response derived directly from its definition, and so does not depend on the kind of system under study. It is easy to check from equations (9) and (17) that this holds for the free Fermi gas.

Figures 1,2 and 3 show the total response of the free Fermi gas and its incoherent and coherent parts at $\tilde{q} = 0.01$, $\tilde{q} = 1$ and $\tilde{q} = 1.9$. The upper plots show the Lindhard function (solid line), while $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$ are drawn below (solid and dashed lines, respectively). There are three main regions at $\tilde{q} \leq 2$ where the Lindhard function changes its behavior due to the different $\tilde{\omega}$ dependence of $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$. At negative $\tilde{\omega}$'s lying between $\tilde{q}^2 - 2\tilde{q}$ and 0, $S_{inc}(\tilde{q}, \tilde{\omega}) = -S_{coh}(\tilde{q}, \tilde{\omega})$ and the total response vanishes. At positive energies smaller than $2\tilde{q} - \tilde{q}^2$, the addition of the two responses cancel the terms quadratic in $\tilde{\omega}$ (see Equations (9) and (17)) and the total $S(\tilde{q}, \tilde{\omega})$ is linear. Finally, at $\tilde{q}^2 + 2\tilde{q} \geq \tilde{\omega} \geq 2\tilde{q} - \tilde{q}^2$ the coherent response vanishes and the dynamic structure function becomes entirely incoherent and quadratic in $\tilde{\omega}$. Out of these limits all three functions are zero.

The different behavior of $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$ is also reflected in figures 1–3. At very low values of the momentum transfer, both $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$ are large, but strong cancelations produce the strength of the total $S(\tilde{q}, \tilde{\omega})$ to be drastically reduced. Notice that in this limit the region $\tilde{\omega} \in (2\tilde{q} - \tilde{q}^2, \tilde{q}^2 - 2\tilde{q})$ where $S(\tilde{q}, \tilde{\omega})$ has only incoherent contributions covers a range $\Delta\tilde{\omega} = 2\tilde{q}^2 \ll 1$, which is much smaller than the range where the two responses coexist. As a consequence, $S(\tilde{q}, \tilde{\omega})$ looks linear in $\tilde{\omega}$ (see figure 1). When $\tilde{q}$ increases, as seen in figure 2, both $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$ are spread and quenched, but the former still shows a maximum well centered at $\tilde{\omega} = \tilde{q}^2$ and the latter a minimum at $\tilde{\omega} = 0$. The minimum of the coherent response coincides with the point where the two functions defined in Eq. (17) join ($\tilde{\omega} = 0$), and the different value between the left and right derivatives at that point produces a peak that sharpens with increasing $\tilde{q}$. At $\tilde{q} = 1$ the range where the coherent response is non–zero becomes maximal, going from $\tilde{\omega} = -1$ to $\tilde{\omega} = 1$, but the incoherent response has a wider range of

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existence, and the total $S(\tilde{q}, \tilde{\omega})$ presents two well differentiated regions, one linear and another quadratic in $\tilde{\omega}$. As $\tilde{q}$ rises above this value, $S_{coh}(\tilde{q}, \tilde{\omega})$ reduces both its magnitude and its range of definition and, in particular, at $\tilde{q} = 1.9$ becomes much smaller than $S_{inc}(\tilde{q}, \tilde{\omega})$ (see figure 3), thus producing a total $S(\tilde{q}, \tilde{\omega})$ that is mostly incoherent.

Another useful tool in the study of the dynamic structure function are the energy weighted sum rules, which can be also derived for $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$. They are defined to be the moments of the different responses

$$m^{(\alpha)}_{inc,(coh)}(\tilde{q}) = \int_{-\infty}^{\infty} d\tilde{\omega}\, \tilde{\omega}^{\alpha} S_{inc,(coh)}(\tilde{q}, \tilde{\omega}) \tag{18}$$

$$m^{(\alpha)}(\tilde{q}) \equiv m^{(\alpha)}_{inc}(\tilde{q}) + m^{(\alpha)}_{coh}(\tilde{q}) = \int_{0}^{\infty} d\tilde{\omega}\, \tilde{\omega}^{\alpha} S(\tilde{q}, \tilde{\omega}) \tag{19}$$

and, even though $m^{(\alpha)}_{inc}(\tilde{q})$ and $m^{(\alpha)}_{coh}(\tilde{q})$ integrate over all energies, $m^{(\alpha)}(\tilde{q})$, built from their sum, is an equivalent integral of the total $S(\tilde{q}, \tilde{\omega})$ but obviously restricted to positive energies.

The first moments read

$$m^{(0)}_{inc}(\tilde{q}) = 1 \tag{20}$$

$$m^{(0)}_{coh}(\tilde{q}) = S(q) - 1 \tag{21}$$

$$m^{(1)}_{inc}(\tilde{q} = \tilde{q}^2 \tag{22}$$

$$m^{(1)}_{coh}(\tilde{q}) = 0 \tag{23}$$

and are the same in a correlated system replacing $S(q)$ by the appropriate static structure factor. For the free Fermi gas, all odd moments of $S_{coh}(\tilde{q}, \tilde{\omega})$ cancel due to the symmetry of the coherent response around $\tilde{\omega} = 0$, while even ones are related to derivatives of ρ_2. Furthermore, as $S_{inc}(\tilde{q}, \tilde{\omega})$ is entirely given by the impulse approximation, all odd order incoherent moments centered at $\tilde{\omega} = \tilde{q}^2$ vanish. Particle correlations in realistic systems may cause the static structure factor to be greater or smaller than 1 as a function of q, as happens in liquid helium. Even though this change in the sign of $m^{(0)}_{coh}(q)$ can be obtained from a $S_{coh}(q, \omega)$ symmetric around $\omega = 0$ that has no nodes, it seems more reasonable to think about a coherent response that has at least one point where the function changes sign, located in such a way that both $m^{(0)}_{coh}(q)$ and $m^{(1)}_{coh}(q)$ are fulfilled. Therefore, this difference in the behavior of the zero moment points towards a change in the structure of the coherent response entirely induced by particle correlations.

The contributions of $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$ at $\tilde{\omega} < 0$, moments (20) to (23) differ from

those obtained integrating over positive energies only. In particular for the Fermi sea, the first moments of $S_{inc}(\tilde{q},\tilde{\omega})$ integrated at $\tilde{\omega} > 0$ are

$$\int_0^\infty d\tilde{\omega}\, S_{inc}(\tilde{q},\tilde{\omega}) \;=\; 1 - \frac{3}{2}\int_{\tilde{q}/2}^\infty \tilde{k}\left(\tilde{k}-\frac{\tilde{q}}{2}\right) n(\tilde{k})\, d\tilde{k} \tag{24}$$

$$\int_0^\infty d\tilde{\omega}\, \tilde{\omega} S_{inc}(\tilde{q},\tilde{\omega}) \;=\; \tilde{q}^2 + \frac{3\tilde{q}}{4}\int_{\tilde{q}/2}^\infty \tilde{k}\left(\tilde{k}-\frac{\tilde{q}}{2}\right)^2 n(\tilde{k})\, d\tilde{k} \tag{25}$$

and coincide with the previous ones at $\tilde{q} > 2$ where $S(\tilde{q},\tilde{\omega}) = S_{inc}(\tilde{q},\tilde{\omega})$ The residual terms appearing in the right hand side of equations (24) and (25) are the manifestation of the negative energy contributions, and are the same in realistic systems when the incoherent response is described by the impulse approximation. Notice that in such systems the momentum distribution $n(k)$ extends up to infinity, and so those terms contribute no matter how large $\tilde{q}$ is. Nevertheless, $n(k)$ decreases rapidly with k and they become vanishingly small as $\tilde{q}$ increases.

In summary, a direct calculation of the coherent and incoherent density responses of the free Fermi gas has revealed significant differences between them and with respect to the total dynamic structure function. While the latter is known to be non–zero and positive at $\omega > 0$ only, none of those constrains apply to the coherent and incoherent responses separately. In particular, and for the Fermi gas, $S_{coh}(q,\omega)$ is negative and symmetric around $\omega = 0$ and both $S_{inc}(q,\omega)$ and $S_{coh}(q,\omega)$ present non–negligible contributions at $\omega < 0$ that cancel exactly once added up. This cancellation also holds in any realistic system. This behavior is also reflected in the energy weighted sum rules.

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Figure captions

Figure 1. Comparison between the dimensionless Lindhard Function (solid line above) and the dimensionless incoherent and coherent dynamic structure functions (solid and dashed lines below, respectively) at $\tilde{q} = 0.01$.

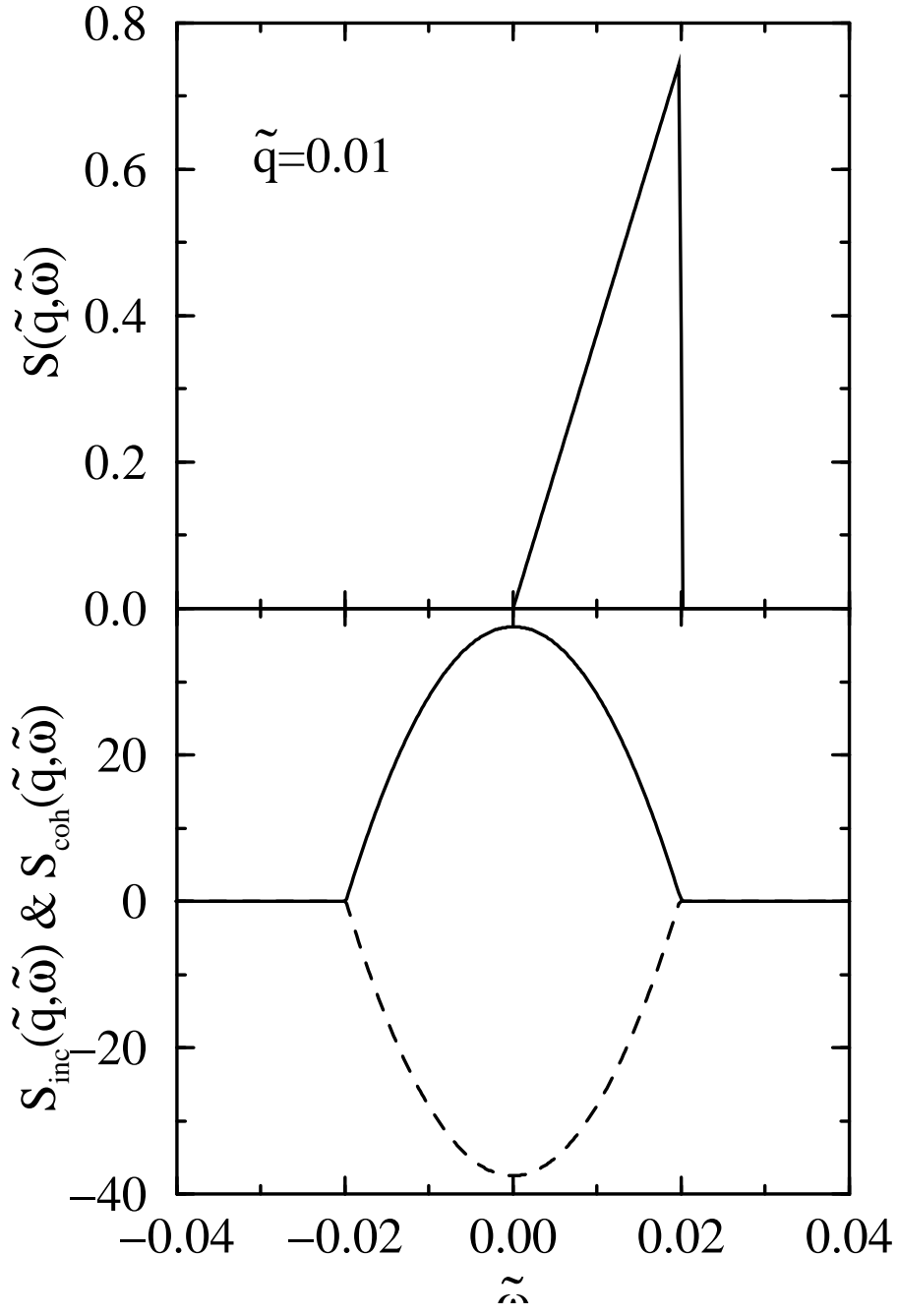**Figure 2.** Same as in figure 1 at $\tilde{q} = 1$.

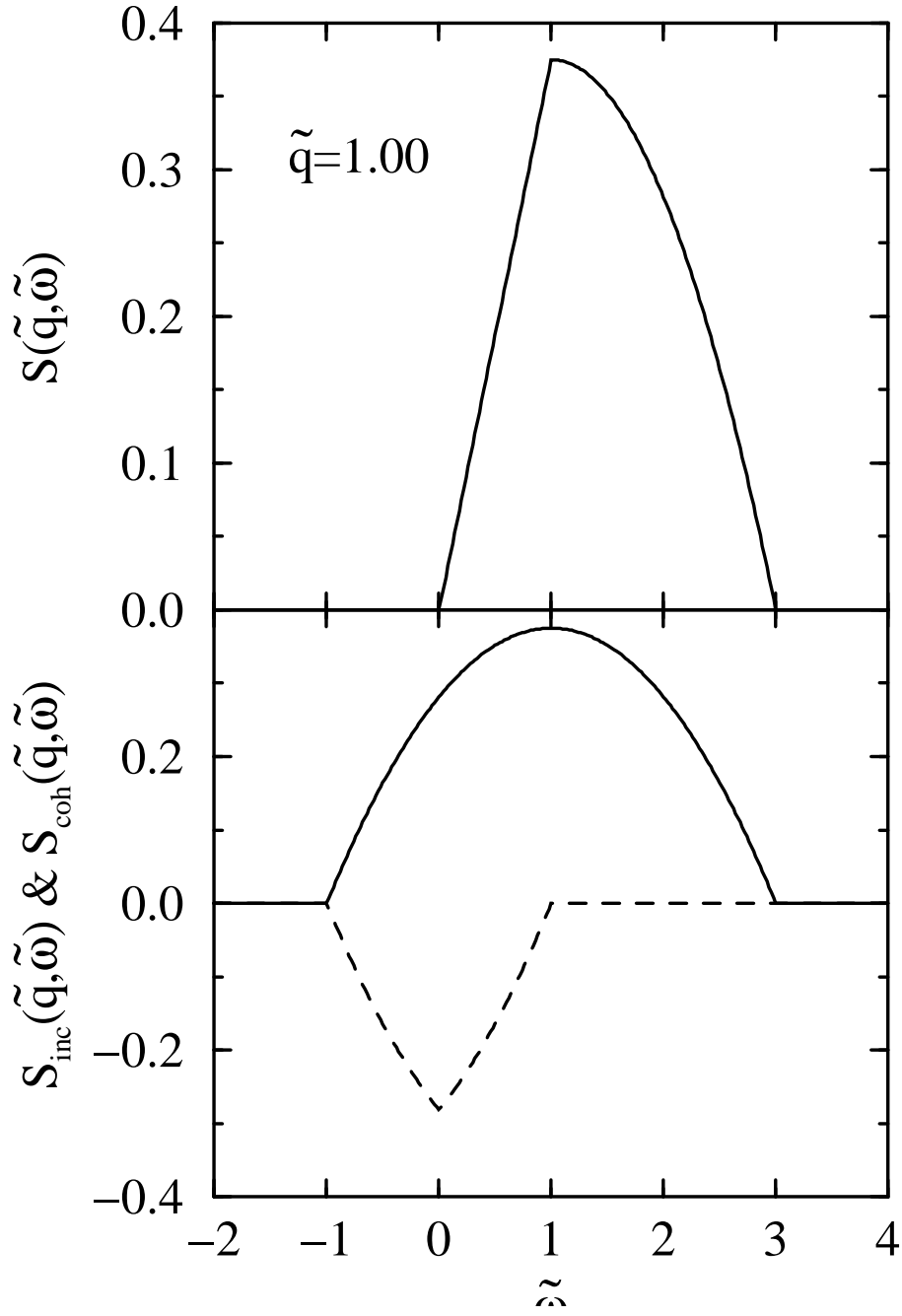**Figure 3.** Same as in figure 1 at $\tilde{q} = 1.9$.

Figure 1:

Figure 2:
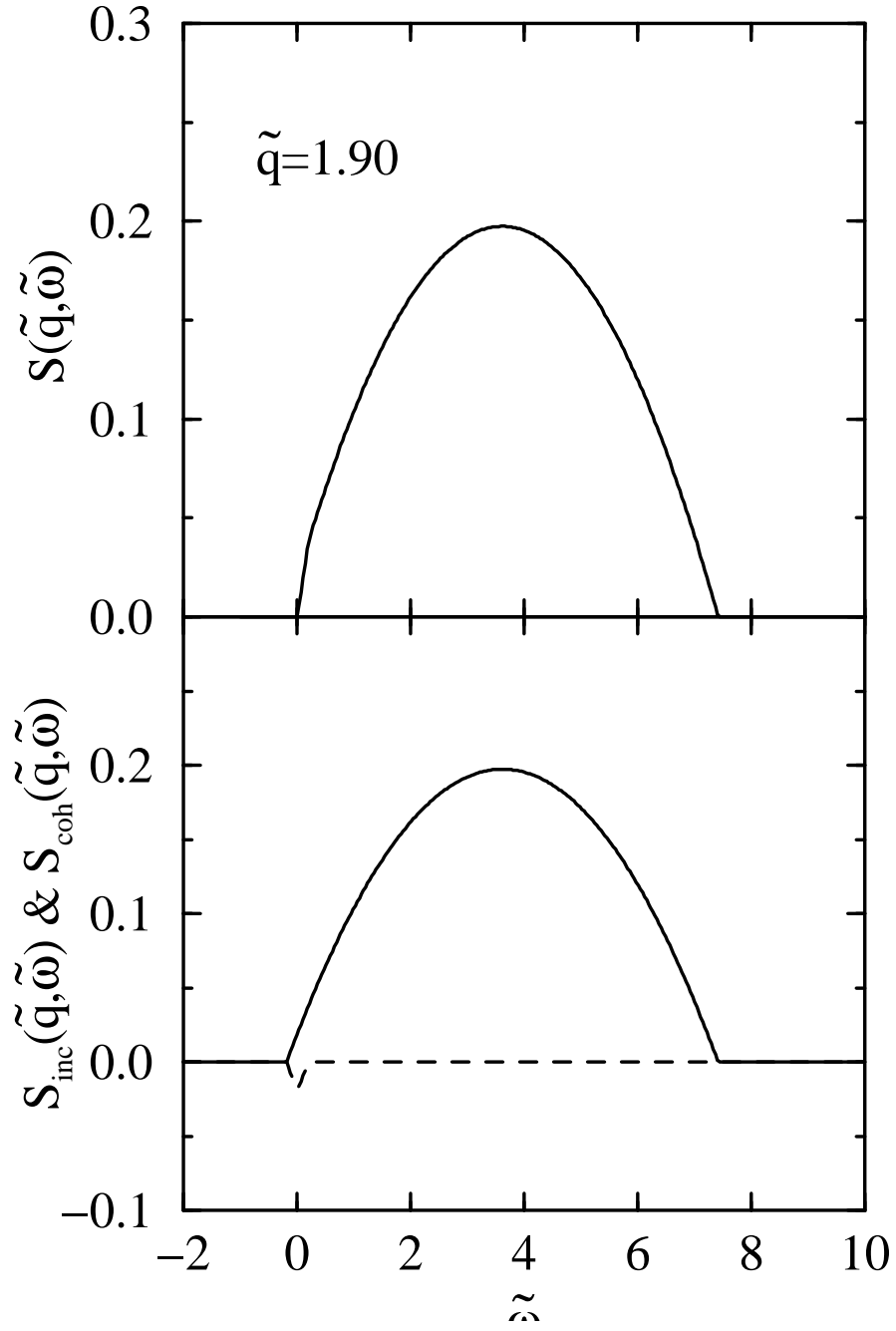
Figure 3: